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6. AUTHOR(S) Zhigang Suo				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Princeton University Department of Mechanical & Aerospace Engineering Princeton, NJ 08544			8. PERFORMING ORGANIZATION REPORT NUMBER	
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Final Report on Related ONR Projects

Zhigang Suo

Mechanical and Aerospace Engineering Department and the Princeton Materials Institute
Princeton University, Princeton, NJ 08544

Grant / Contract Title: INVESTIGATIONS ON DEGRADATION MECHANISMS FOR
FERROELECTRIC ACTUATOR DESIGN

Performing Organization: University of California, Santa Barbara

Principal Investigator: Zhigang Suo

Contract Number: N00014-93-1-0110

ONR Scientific Officer: Dr. Roshdy Barsoum

Grant / Contract Title: RESEARCH IN RELIABILITY OF CERAMIC ACTUATORS

Performing Organization: University of California, Santa Barbara and Princeton University

Principal Investigator: Zhigang Suo

Contract Number: N00014-97-1-0260 (to UCSB)

Contract Number: N00014-97-1-1028 (Transferred to Princeton)

ONR Scientific Officer: Dr. Roshdy Barsoum

Research Objectives

Among various materials for solid state actuators (e.g., magnetostrictors, shape memory alloys, and ferroelectric ceramics), ferroelectric ceramics are most versatile, offering a combination of large actuation work per unit volume, fast response, low cost, and electric field control. Ferroelectrics have long been used in non-structural applications (e.g., pressure sensors, microphones) that require small forces and displacements. Their brittleness has not been the limiting factor in such applications. Recent applications include large-scale adaptive structures, active vibration control, and precise positioning, all requiring large actuation work under repeated loading. Although each application involves many technical issues (e.g., sensing, signal processing, actuation, structural design), it is the reliability of actuators that has become the limiting factor.

The present actuator design practice is empirical: no data base and analytical tool exist to assure long term reliability. This is in contrast with most other structural elements, where years of experience and research have accumulated such data bases and tools. Often it is this lack of reliability assurance that stands in the way of integrating actuators into structures. The object of the proposed research is to create a computational tool to design reliable actuators. The work focuses on multilayer actuators, although ideas and tools to be developed would be relevant to other types of actuators.

Technical Approach and Accomplishments

Most reliability problems relate to internal stresses in the actuators. In nearly all actuator designs, the internal electrodes have geometric discontinuities (e.g., internal electrode edges), around which the applied voltage induces a nonuniform electric field. The nonuniform electric field induces internal stresses. Cracks can nucleate near electrode edges, and grow under cyclic voltage. Apparently, such cracks do not change mechanical performance significantly. However, a crack, once connects electrodes of opposite polarity, provides an easy electrical breakdown path.

Because ceramic layers in an actuator are connected in parallel, one breakdown site would cause short circuit and the whole device would cease to function.

The above sequence of events, or its variants, identifies cracking as a prerequisite for electrical breakdown. The voltage required to cause breakdown by this process can be much smaller than that required in the absence of cracks. The general strategy to avoid cracking is to change materials or electrode configuration to reduce internal stresses. Such changes, of course, are subject to the constraint of cost and performance. We have developed a crack nucleation model under the small-scale saturation conditions. This model shows that, for a given actuator material and electrode configuration, crack will not nucleate if the individual ceramic layer is below a critical thickness. Such dependence on layer thickness is qualitatively consistent with the available experience.

We have developed a finite element program to solve the coupled, nonlinear electromechanical problem. At present, the material is taken to be nonlinear dielectric with electrostrictive strain quadratic in elastic displacement. We have used the program to solve field distribution in a multilayer actuator, which are then combined with fracture mechanics to obtain cracking condition. The calculations are compared with the above analytical solution under the small-scale saturation conditions, and then extended to the large-scale saturation conditions. We have shown that the cracking condition established under the small-scale saturation conditions gives useful estimates even when the saturation zone is comparable to the actuator layer thickness. We have also used the program to compare actuators of different designs, such as those with or without edge slits. We show that the slits do not significantly reduce the stresses near the electrode edge. However, they do reduce stress over a larger volume in the insulating gap.

The PI has published a critical review of the current understanding of the effects of stress and strain, with particular emphasis on small structures, such as cracking in multilayer actuators, thin films, and small particles.

(Ba,Sr)TiO₃ films on silicon substrates are being developed for dynamic random access memories. These films are under large tensile stresses due to deposition process and thermal

expansion misfit. By a converse electrostrictive effect, a tensile stress in the plane of the film reduces the capacitance measured through the thickness of the film. Tom Shaw and I are finishing a paper reporting our effort to quantify this effect. The residual stress in a film was determined by measuring the change in the substrate curvature upon the removal of the film. In a separate experiment, a force was applied to vary the stress in a film on a wafer, and the change in the capacitance of the film was recorded. The data allowed us to infer the electrostrictive coefficient of the film, and the capacitance of a stress-free film. The methods developed are applicable to evaluate the stress effect on any high-permittivity solid films.

Relevance To Navy

Large strain actuators have many applications. Cracking in actuators near electrode edges has been a long standing problem. There is a basic dilemma. Large strains are desired for actuator applications. A recent emphasis of the program at PENN State supported by ONR is to develop materials with larger strains. On the other hand, such larger strains induce more incompatibility around electrode edges. Our work shows that if one makes layer thickness and insulation gap small enough, even large-strain actuator will not crack. Our finite element calculations can provide design rules in developing actuators of new materials and geometry.

List of Publications /Reports / Presentations

1. Papers Published in Refereed Journals

- Z. Suo, "Models for breakdown-resistant dielectric and ferroelectric ceramics," *J. Mech. Phys. Solids*, **41**, 1155-1176 (1993).
- W. Yang and Z. Suo, Cracking in ceramic actuators caused by electrostriction. *J. Mech. Phys. Solids*, **42**, 649-664 (1994)
- W. Pompe, X. Gong, Z. Suo and J.S. Speck, Elastic energy release due to domain formation in the strained epitaxy of ferroelectric and ferroelastic films. *J. Appl. Phys.* **74**, 6012-6019 (1993).
- T.H. Hao, X. Gong and Z. Suo, "Fracture mechanics for the design of ceramic multilayer actuators," *J. Mech. Phys. Solids*, **44**, 23-48 (1996).
- R.E. Loge and Z. Suo, "Nonequilibrium thermodynamics of ferroelectric domain evolution," *Acta Materialia*, **44**, 3429-3438 (1996).
- X. Gong and Z. Suo, "Reliability of ceramic multilayer actuators: a nonlinear finite element simulation," *J. Mech. Phys. Solids*, **44**, 751-769 (1996).
- C. Hillman, Z. Suo, F.F. Lange, "Cracking of laminates subjected to biaxial tensile stresses," *J. Am. Ceram. Soc.* **79**, 2127-2133 (1996).
- Z. Suo and H. Yu, "Crack nucleation on elastic polycrystal surface in corrosive environment: low dimensional dynamical models," *Acta Materialia* 2235-2245, **45** (1997).
- Z. Suo, Stress and strain in ferroelectrics. *Current Opinion in Solid State & Materials Science*, **3**, 486-489 (1998).
- T.M. Shaw, Z. Suo, M. Huang, E. Liniger, R.B. Laibowitz, J.D. Baniecki, "The effect of stress on the dielectric properties of barium strontium titanate thin films". Submitted to *Appl. Phys. Lett.*.
- Z. Suo, "Evolving small structures," Prepared for *Research Trends in Solid Mechanics*, a volume coordinated by G.J. Dvorak on behalf of The U.S. National Committee on Theoretical and Applied Mechanics.
- H. Yu and Z. Suo, "A model of wafer bonding by elastic accommodation," *J. Mech. Phys. Solids* **46**, 829-844 (1998).

2. Non-Refereed Publications

- X. Gong and Z. Suo, "A nonlinear finite element method for electrostrictive ceramic multilayer actuators—a comparison of capacitor-type and slit structures," The Minerals, Metals and Materials Society (TMS) Proceedings.
- X. Gong, H. Yu, Z. Suo and R.M. McMeeking, "Cracking in ferroelectric and antiferroelectric ceramic multilayer actuators." Proceedings of the ASME Aerospace Division. AD-Vol. 52. P703-712. Edited by Xhang, J.C.I., Coulter, J., Brei, D., Martinez, D., Ng, W., Freidmann, P.P.

3. Presentations

a. Invited

- February 1997 "Reliability of ferroelectric ceramic multilayer devices," TMS Annual Meeting, Orlando, Florida.
- April 1997 "Design against cracking in microstructures," Component Research, Intel, Santa Clara, CA.
- April 1997 "Crack-proof small structures," Acta Materialia Workshop on Coupled Property Issues in Integrated Microstructures. Monterey, CA.
- April 1997, "Fail-safe design of ferroelectric actuators," International Smart Actuator Symposium. State College, PA.
- May 1997, "Multiple energetics and kinetics," Campbell Symposium on Dynamics of Microstructure. Ann Arbor, MI.
- September 1997, "Cracking in integrated microstructures," Mechanical and Aerospace Engineering Department, University of Tennessee.
- September 1997 "Morphology selection in materials—case studies," Solid State Division, Oak Ridge National Laboratory.

b. Contributed

- December 1996, "Competitive motions of grain boundary and free surface in selecting thin film morphology," MRS Fall Meeting, Boston.
- February 1997, "Crack Nucleation on Elastic Polycrystal Surfaces in Corrosive Environment," TMS Annual Meeting, Orlando, Florida.
- March 1997 "Reliability of ferroelectric ceramic multilayer devices," Smart Structures and Materials Symposium, San Diego.

March 1997 "Dislocation dynamics in electron wind," Workshop on Dislocation and Plasticity,
Institute of Theoretical Physics, Santa Barbara.

4. Book Sections

Z. Suo, "Motions of microscopic surfaces in materials," *Advances in Applied Mechanics*.
Vol. **33** 193-294 (1997).

Awards and Honors Received by the PI (Z. Suo)

Pi Tau Sigma Gold Medal "for outstanding achievement in mechanical engineering within ten years
of graduation", American Society of Mechanical Engineers, 1994.

Alexander von Humboldt Research Fellowship, Germany, 1994.

Participants

Z. Suo, Professor, PI.

W. Yang, Professor, Visiting Researcher.

C.L. Lynch, Post-doc.

X. Gong, Graduate Student.

R. Loge, Graduate Student.

M. Huang, Graduate Student